

Stochastic Split Determinant Algorithms

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I propose a large class of stochastic Markov processes associated with probability distributions analogous to that of lattice gauge theory with dynamical fermions. The construction incorporates the idea of approximate spectral split of the determinant through local loop action, and the idea of treating the infrared part of the split through explicit diagonalizations. I suggest that *exact algorithms* of practical relevance might be based on the Markov processes so constructed.

One of the difficulties we face in lattice gauge theory is how to efficiently simulate the gauge invariant distribution

$$P(U) \propto e^{-S_B(U)} \det M(U) \equiv P_1(U)P_2(U) \quad (1)$$

with bounded bosonic action $S_B(U)$, and the fermionic kernel $M(U)$, such that $\det M(U) \geq 0$.

The dynamic Monte Carlo approach, which is usually adopted, is based on identifying a suitable ergodic Markov process, defined by the Markov matrix $T(U, U')$, which has required distribution as a fixed point, i.e. $\int dU P(U)T(U, U') = P(U')$. While finding examples of valid Markov processes is by no means difficult, finding a *suitable* one proved to be a formidable task.

In the discussion that follows, I will construct Markov processes built on rather different ingredients than those of established methods. They incorporate several interesting ideas that appeared in recent years, and the corresponding *exact algorithms* have a chance of being reasonably practical, while perhaps being more accommodative of complicated actions of Ginsparg-Wilson type. The main influence in the construction I will present is the method used in the inexact Truncated Determinant Algorithm (TDA) [1].

Probability distribution that splits into two unnormalized products such as (1) can in principle be simulated using the following statement. Let $T_1(U, U')$ be the Markov matrix satisfying detailed balance with respect to P_1 , i.e. $P_1(U)T_1(U, U')dU = P_1(U')T_1(U', U)dU'$, and

*Work supported in part by the DOE under grant No. DE-FG02-97ER41027.

let $P_2^{acc}(U, U') = \min[1, \frac{P_2(U')}{P_2(U)}]$ be the Metropolis acceptance probability with respect to P_2 . Then the transition matrix

$$T(U, U') \equiv T_1(U, U')P_2^{acc}(U, U'), \quad U \neq U' \quad (2)$$

satisfies detailed balance with respect to the distribution $P \propto P_1P_2$. Consequently, T represents a valid Markov process assuming T_1 is ergodic.

While there is a lot of freedom in choosing the process T_1 , the algorithm based on T very much exemplifies the difficulties associated with simulating distribution (1). For one, the calculation of acceptance probability requires the calculation of determinant ratio, which is hard. Also, if T_1 represents the probabilities for the sweep of suitable local changes, for example, then the determinant is expected to fluctuate strongly, giving rise to severe problems with equilibration and, hence, useless algorithm. Nevertheless, this is a natural starting point and the aim is to improve upon these bad things.

As a first point to notice, there is an additional significant freedom in the above procedure. In particular, it is possible to split the distribution (1) in two parts in infinitely many ways by multiplying and dividing with arbitrary bounded positive function of the gauge fields, i.e.

$$P_1(U) = e^{-S_B - \Delta S_B} \quad P_2(U) = e^{\Delta S_B} \det M \quad (3)$$

Labeling the splits by ΔS_B , we thus have a family of Markov processes $T[\Delta S_B]$ constructed as in (2), each with the correct fixed point.

The reason why this can be useful is implicitly contained in the well established fact, that if the

fermions are not very light, the effects of the determinant can be absorbed in the simple shift of the gauge coupling [2]. This suggests that one can follow the fluctuations of the determinant in such a case by approximating it with a simple loop action. Using such an action for the split ΔS_B as described above can therefore presumably reduce the fluctuations of the determinant part substantially even if the fermions are not heavy. Analogous observations in more or less related contexts were made for example in Refs. [3–5].

Supposing this works, we are still left with an awkward algorithm, because the evaluation of Metropolis acceptance probability is costly. One way to proceed is to consider the stochastic linear Kennedy-Kuti acceptance probability instead [6], which can be cheap for the price of introducing some extra noise. Indeed, we can generalize the transition matrices (2) to stochastic ones and use the following statement. Let $T_1(U, U')$ be the Markov matrix satisfying detailed balance with respect to P_1 . Let further $\hat{R}_a(U, U')$ be a stochastic estimator, depending on the set of stochastic variables a , so that $\langle \hat{R}_a(U, U') \rangle_a = P_2(U')/P_2(U)$, and let

$$\hat{P}_{2,a}^{acc} = \begin{cases} \lambda_+ + \lambda_- \hat{R}_a(U, U'), & \text{if } U > U'; \\ \lambda_- + \lambda_+ \hat{R}_a(U, U'), & \text{if } U < U', \end{cases} \quad (4)$$

where λ_+, λ_- are constants and some ordering of the gauge fields is assumed. If we define

$$\hat{T}_a(U, U') \equiv T_1(U, U') \hat{P}_{2,a}^{acc}(U, U'), \quad U \neq U' \quad (5)$$

then $T(U, U') = \langle \hat{T}_a(U, U') \rangle_a$ satisfies detailed balance with respect to $P \propto P_1 P_2$. Consequently, the stochastic transition matrices (5) can serve to generate a valid Markov sequence assuming that T_1 is ergodic and the individual estimates $\hat{P}_{2,a}^{acc}$ can be interpreted as probabilities.

With this framework in mind, we are now dealing with large class of stochastic matrices $\hat{T}[\Delta S_B, \hat{P}_{2,a}^{acc}]$ that are assigned to $P(U)$ and, in addition to the choice of split action, are also labeled by the choice of stochastic probability estimator. The challenge now is to construct an estimator that is (a) reasonably cheap, (b) does not require too much noise so that the fluctuations already reduced by the split will not come back,

(c) introduces negligible amount of probabilistic violations in the acceptance step.

That this can be done in the useful novel way is suggested by the qualitative observation that the small eigenvalues of the lattice Dirac operator contribute substantially to the long distance behaviour of the effective fermionic action while large eigenvalues are more relevant at short distances [1]. This obviously makes very good physical sense, but it should be said that to make more quantitative statements appears to be non-trivial. Nevertheless, it suggests that after the fluctuations of the full determinant are reduced by splitting the distribution with some ultralocal loop action, what is left in the determinant part is dominated by small eigenvalues. We should thus construct an estimator $\hat{R}_a(U, U')$ entering (4) that assumes bulk contribution from small eigenvalues, thus being able to take advantage of the approximate spectral split.

Such an estimator can be constructed as follows. By definition, we need to estimate the quantity $R(U, U') = P_2(U')/P_2(U)$. If λ_i denote the eigenvalues of $M(U)$, this can be written as

$$\frac{e^{\Delta S_B(U')} \lambda'_1 \lambda'_2 \dots \lambda'_N}{e^{\Delta S_B(U)} \lambda_1 \lambda_2 \dots \lambda_N} \equiv x_1 x_2 \dots x_N, \quad (6)$$

where $x_i \equiv \frac{\lambda'_i}{\lambda_i} e^{[\Delta S_B(U') - \Delta S_B(U)]/N}$, and the eigenvalues are assumed to be ordered by increasing magnitude. The monomial can then be estimated by

$$\begin{aligned} \hat{R}_a &= x_1 + \hat{a}_1 \frac{x_1}{\alpha_1} (x_2 - 1) + \\ &+ \hat{a}_1 \hat{a}_2 \frac{x_1 x_2}{\alpha_1 \alpha_2} (x_3 - 1) + \dots \\ &+ \hat{a}_1 \hat{a}_2 \dots \hat{a}_{N-1} \frac{x_1 x_2 \dots x_{N-1}}{\alpha_1 \alpha_2 \dots \alpha_{N-1}} (x_N - 1), \end{aligned} \quad (7)$$

where $0 < \alpha_i \leq 1$ and \hat{a}_i are independent random variables distributed according to

$$\hat{a}_i = \begin{cases} 1, & \text{with probability } \alpha_i; \\ 0, & \text{with probability } 1 - \alpha_i. \end{cases} \quad (8)$$

Obviously, one has $\langle \hat{R}_a \rangle_a = x_1 x_2 \dots x_N$ as desired, and it is useful to emphasize the following points:

(A) It is trivial to generate \hat{a}_i by using the random number generator. To get \hat{R}_a , one can first

assign to it the value x_1 and generate \hat{a}_1 . If \hat{a}_1 is zero, this is the whole estimate because \hat{a}_1 multiplies all the remaining terms. If \hat{a}_1 is one, the second term is added and \hat{a}_2 is generated. Again, if \hat{a}_2 is zero, the estimate is completed and if it is one, the third term is added and \hat{a}_3 generated etc. The calculation stops as soon as the first \hat{a}_i is zero, and only the corresponding number of smallest eigenvalues is needed. The required number of eigenvalues can be determined beforehand if desired, and the average number over many estimates can be tuned by changing $\{\alpha_i\}$.

(B) One can group the contributions of several eigenvalues into a single variable x_i , and the number of eigenvalues so grouped does not have to be the same for all x_i . For example, if the split action ΔS_B is determined by fitting the ultraviolet part of the truncated determinant [7], then it is probably best to group into x_1 the smallest eigenvalues almost up to the truncation number, and group the remaining eigenvalues differently so that the stochastic part of \hat{R}_a does not fluctuate a lot.

(C) Strictly speaking, λ_i do not have to be the eigenvalues of M . For example, in case of two flavours of Wilson fermions, we can instead use $\lambda_i = \delta_i^* \delta_i$, where δ_i are the eigenvalues of one flavour operator. It is in fact desirable that the corresponding x_i be real non-negative and so, if the individual eigenvalues are not, we assume that we can group them together so that the resulting product is, or use additional properties such as in the example above. This is possible in situations of practical interest.

(D) The amount of noise introduced by the estimator (7) is typically much less than with the traditional $e^{Tr \log M}$ estimators, and can be tuned by changing the values $\{\alpha_i\}$. This comes at the price of calculating the lowest eigenvalues.

For obvious reasons, it is natural to call the algorithms based on $\hat{T}[\Delta S_B, \hat{P}_{2,a}^{acc}]$ of (5) with the estimator of type (7) the Stochastic Split Determinant Algorithms (SSDA). They simultaneously use the complementary representations of effective fermionic action in terms of gauge loops with increasing length (converging rapidly at small distances), and in terms of Dirac eigenvalues with increasing magnitude (converging rapidly at large distances). If the two representations overlap suf-

ficiently with small number of terms, then a simple split action ΔS_B can be found and T_1 , $\hat{P}_{2,a}^{acc}$ easily adjusted, so that the number of probabilistic exceptions is negligible, and efficient *exact* SSDA results. The TDA work [1,7] suggests that this might be the case for reasonably large lattices in QCD_4 . The work on quantitative aspects of these statements is in progress and will be reported elsewhere.

On sufficiently large lattices, algorithms like TDA or SSDA in their current form will eventually have inferior efficiency to that of HMC, which has more favourable volume scaling. However, the crucial advantage of TDA and SSDA is that they essentially treat fermions in the eigenspace of operator M . As such, they are in principle applicable to functions $f(M)$ as well. For example, simulations of two or arbitrary flavours of staggered fermions is straightforward here.

Finally, it should be emphasized that in the current context, the underlying process T_1 can always be chosen so that there will essentially be no exceptions at all. In bad cases this can rapidly increase the work per independent configuration, but exactness can always be achieved. However, the underlying philosophy appears to be sufficiently solid to believe that the framework is large enough for some practically relevant algorithms to be found here.

I thank Hank Thacker for many pleasant discussions on the topics presented here.

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